

Benzamide, 3-bromo-N-butyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C19H30BrNO/c1-4-7-10-16(6-3)15-21(13-8-5-2)19(22)17-11-9-12-18(20)14-17
InchiKey:	HASZMZNMWDDDDAS-UHFFFAOYSA-N
Formula:	C19H30BrNO
SMILES:	CCCCC(CC)CN(CCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	368.35

Physical Properties

Property code	Value	Unit	Source
gf	205.62	kJ/mol	Joback Method
hf	-234.43	kJ/mol	Joback Method
hfus	45.00	kJ/mol	Joback Method
hvap	75.66	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.908		Crippen Method
mvol	283.860	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rmpol	2933.00		NIST Webbook
rmpol	2933.00		NIST Webbook
tb	797.81	K	Joback Method
tc	1001.82	K	Joback Method
tf	470.03	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.31	J/molxK	797.81	Joback Method
cpg	844.36	J/molxK	831.81	Joback Method
cpg	860.37	J/molxK	865.81	Joback Method
cpg	875.40	J/molxK	899.82	Joback Method
cpg	889.52	J/molxK	933.82	Joback Method
cpg	902.80	J/molxK	967.82	Joback Method
cpg	915.30	J/molxK	1001.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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